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NONEXISTENCE OF SLOW HETEROCLINIC TRAVELLING WAVES FOR A BISTABLE HAMILTONIAN LATTICE MODEL

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ABSTRACT. The nonexistence of heteroclinic travelling waves in an atomistic model for martensitic phase transitions is the focus of this study. The elastic energy is assumed to be piecewise quadratic, with two wells representing two stable phases. We demonstrate that there is no travelling wave joining bounded strains in the different wells of this potential for a range of wave speeds significantly lower than the speed of sound. We achieve this using a profile-corrector method previously used to show existence of travelling waves for the same model at higher subsonic velocities.

1. INTRODUCTION

Is it possible for an elastic solid to exhibit a slowly-moving phase boundary? We address this question using a Fermi-Pasta-Ulam (FPU) chain to model the material, which is a one-dimensional bi-infinite chain of identical point unit masses, representing atoms, joined to their nearest neighbours with springs. When modelling phase transitions, the springs typically have a nonconvex stored energy potential with different wells representing the different stable phases. Here we study materials with two distinct stable phases. This model with piecewise quadratic interactions was studied analytically and numerically by Balk *et al.* [2, 3].

The formulation is as follows. Let $u_j(t) \in \mathbb{R}$ be the displacement of the j th atom with respect to the uniform reference configuration \mathbb{Z} at time $t \in \mathbb{R}$. Denoting the potential function as $V: \mathbb{R} \rightarrow \mathbb{R}$ and assuming that the evolution of the dynamics is governed by Newton's second law, one finds that the equation of motion is

$$(1) \quad \ddot{u}_j(t) = V'(u_{j+1}(t) - u_j(t)) - V'(u_j(t) - u_{j-1}(t)), \quad j \in \mathbb{Z}.$$

A solution of (1) is a *travelling wave* if it has the form

$$(2) \quad u_j(t) = u(j - ct), \quad j \in \mathbb{Z}$$

where the constant c is the wave speed. We say that a travelling wave solution represents a *phase transition* in the material if it has strains in both wells of the potential. Furthermore, a travelling wave representing a phase transition is *heteroclinic* if it asymptotically belongs to different wells. Such phase transitional travelling waves were first studied using Fourier analysis for a FPU chain with piecewise quadratic interaction potential by Truskinovsky and Vainchtein [14]. Schwetlick and Zimmer propose [8] an alternative framework to address the existence of subsonic phase transition waves very close to the speed of sound. The speed of sound is defined as $c_0 := \sqrt{V''}$. Here we show that this framework, although used to prove existence, can be adapted to prove a seemingly contrary proposition, the nonexistence of single transition waves for a slow wave speed regime.

The question of what happens at subsonic wave speeds significantly lower than the speed of sound has, to the best of our knowledge, not been addressed in an analytical framework before. It has been conjectured by Peyrard and Kruskal [7] that travelling waves with low constant wave speeds do not exist for the related Frenkel-Kontorova model on finite domains. Here we show this conjecture is true for the bi-infinite FPU chain as there is no travelling wave joining bounded strains in the different wells of the bilinear potential for wave speeds significantly lower than the speed of sound. Consequently this means that at low subsonic wave speeds there are no phase transitional solutions to the lattice differential equation (1) that makes a single transition between the potential wells. Remarkably, the methods are rather similar to those used to show the opposite result, namely the existence of travelling waves for very fast subsonic waves [8]. Our result indicates that the motions at the low wave speeds considered here may be less coherent than these with speeds close to the speed of sound. It may be possible that there are travelling wave solutions with multiple interfaces, or solutions that are not of travelling wave type. In conjunction with [8], the result presented here describes a dichotomy: coherent single-interface travelling waves exist for high subsonic velocities but not for low velocity. Such a dichotomy between fast and slow martensitic transformations has been observed experimentally by Förster and Scheil [4] in the 1940's.

2. MATHEMATICAL DESCRIPTION

We consider a one-dimensional chain of atoms $\{q_j\}_{j \in \mathbb{Z}} \subset \mathbb{R}$ whose deformations are given as $u_j: \mathbb{R} \rightarrow \mathbb{R}$. We have made the assumption that the dynamics can be described by Newton's second law and that the equations of motion are given by (1).

The motion of the phase boundary can be modelled as a travelling wave with strains in both wells of the potential. With the ansatz (2) the equations of motion (1) reduce to a single equation

$$(3) \quad c^2 u''(x) = V'(u(x+1) - u(x)) - V'(u(x) - u(x-1)).$$

For the analysis of phase transitions in lattice models it is beneficial to reformulate equation (3) in terms of the *discrete strain*. We define the discrete strain as $\varepsilon(x) := u(x) - u(x-1)$ and specify the potential as a function of ε . In this study we consider the potential previously analysed in [2, 3, 8, 14],

$$(4) \quad V(\varepsilon) := \frac{1}{2} \min \{(\varepsilon + 1)^2, (\varepsilon - 1)^2\}.$$

So there are two wells joined at 0 by a cusp and the speed of sound is unity. Having wells at ± 1 is immaterial however it is possible to rescale and translate the potential, as demonstrated by Schwetlick and Zimmer in [10], so that the wells are located at 0 and at a small positive strain. Furthermore, we define the discrete Laplacian to be

$$\Delta_1 f(x) := f(x+1) - 2f(x) + f(x-1).$$

Equation (3) can be now reformulated as the *discrete strain equation*

$$(5) \quad c^2 \varepsilon''(x) = \Delta_1 V'(\varepsilon(x)).$$

Given the explicit form of the potential (4) it is easy to check that (5) becomes

$$(6) \quad c^2 \varepsilon''(x) = \Delta_1 \varepsilon(x) - 2\Delta_1 H(\varepsilon(x)),$$

where

$$(7) \quad H(x) := \begin{cases} 0 & \text{if } x < 0, \\ \frac{1}{2} & \text{if } x = 0, \\ 1 & \text{if } x > 0. \end{cases}$$

Defining the linear operator $L_c := c^2 \partial^2 - \Delta_1$ we rewrite (6) as the following nonlinear advance-delay differential equation

$$(8) \quad L_c \varepsilon(x) = -2\Delta_1 H(\varepsilon(x)).$$

We say that a travelling wave satisfies the *sign condition* or has a *single transition* if it satisfies the property

$$(SC) \quad x \cdot \varepsilon(x) > 0 \text{ for every } x \neq 0.$$

Condition (SC) is central to this paper as it implies that there is exactly one transition between the potential wells, located at the origin in the moving frame coordinates.

The aim of this paper is to demonstrate that there exists a range of values for c , whose absolute values are much less than unity, such that there are no single-transition heteroclinic travelling wave solutions to (8).

3. FOURIER ANALYSIS AND THE DISPERSION RELATION

The Fourier transform of an $L^2(\mathbb{R})$ function $u: \mathbb{R} \rightarrow \mathbb{R}$ is

$$\mathcal{F}[u](\kappa) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u(x) \exp(-i\kappa x) dx, \quad \kappa \in \mathbb{R}$$

where this exists. The Fourier sine transform of u is

$$(9) \quad \mathcal{F}_s[u](\kappa) := \sqrt{\frac{2}{\pi}} \int_0^{\infty} \sin(\kappa x) u(x) dx.$$

Note that the relation $\mathcal{F}[u] = -i\mathcal{F}_s[u]$ holds when u is an odd function.

We define the dispersion relation to be the symbol of the linear operator L_c , which is defined by

$$\mathcal{F}[L_c \varepsilon](\kappa) = D(\kappa) \mathcal{F}[\varepsilon](\kappa),$$

where

$$(10) \quad D(\kappa) := -c^2 \kappa^2 + 4 \sin^2 \left(\frac{1}{2} \kappa \right)$$

is the *dispersion function*. In our notation we suppress the functional dependence of c in D , since our arguments are performed for a fixed value of c^2 . The dispersion relation is given by $D(\kappa) = 0$. It proves convenient to define the function

$$(11) \quad d(\kappa) := \begin{cases} \left(\frac{\sin(\frac{1}{2}\kappa)}{\frac{1}{2}\kappa} \right)^2 & \text{if } \kappa \neq 0, \\ 1 & \text{if } \kappa = 0 \end{cases}$$

so that we can rewrite the dispersion function as $D(\kappa) = (d(\kappa) - c^2)\kappa^2$. As a consequence κ is a zero of the dispersion function if and only if $d(\kappa) = c^2$ or $\kappa = 0$ for any $c \in \mathbb{R}$.

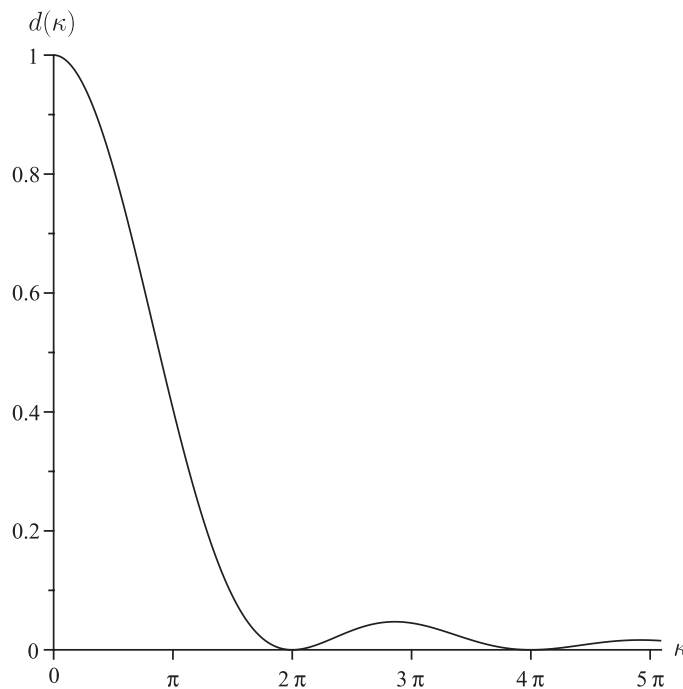


FIGURE 1. Graph of $d(\kappa)$ for $0 \leq \kappa \leq 5\pi$

In this paper we consider values of c for which the equation $d(\kappa) = c^2$ has precisely three roots although in principle these arguments hold for c corresponding to a higher odd number of roots. The case with $c = 0.016$, corresponding to 5 distinct roots, is considered in Section 6. These situations have been studied numerically by Slepyan *et al.* in [12]. Instead of specifying the wave speed directly we prescribe a root of the dispersion

function. This in turn defines the wave speed and the other roots. Let $\hat{\kappa}$ be the value of κ corresponding to the unique maximum of d on $[2\pi, 4\pi]$. Specifically, for $\frac{1}{25} < \rho < \frac{1}{2}$, let $\kappa_1 := \hat{\kappa} - \rho$. We interpret κ_1 as a root of the equation $d(\kappa) = c_\rho^2$ for some wave speed c_ρ . Denote the two other roots of this equation κ_0 and κ_2 , such that $\kappa_0 < \kappa_1 < \kappa_2$. One can estimate numerically that $\hat{\kappa} \approx 8.9868$ to 4 decimal places. Consequently we obtain the numerical bound $8.48 < \kappa_1 < 8.95$. For these values of κ_1 we can estimate the range of values for c_ρ^2 and then use the piecewise monotonicity of d^2 , see Figure 2, to verify that bounds $5.10 < \kappa_0 < 5.12$ and $9.01 < \kappa_2 < 9.51$ hold. In later arguments it will be necessary to refer to these bounds. For simplicity we make the definitions

$$(12) \quad W_0 := (5.10, 5.12), \quad W_1 := (8.48, 8.95) \quad \text{and} \quad W_2 := (9.01, 9.51).$$

The nonexistence result of this paper can be stated as follows.

Theorem 3.1. *For wave speeds c_ρ^2 with $\frac{1}{25} < \rho < \frac{1}{2}$, and V as in (4), there is no travelling wave solving (3) that satisfies the single transition property (SC) and has bounded strain.*

One can estimate numerically, as described above, that the values of c^2 for which Theorem 3.1 holds is $[0.04420, 0.04717]$. Before giving an outline proof we make the following observation. If a function $\varepsilon: \mathbb{R} \rightarrow \mathbb{R}$ satisfies (SC) then

$$(13) \quad f(x) := \Delta_1 H(\varepsilon) = \begin{cases} 1 & \text{for } x \in (-1, 0), \\ -1 & \text{for } x \in (0, 1), \\ 0 & \text{else.} \end{cases}$$

Consequently by assuming the sign condition we may reduce the nonlinear right-hand side of (8) into a function depending just on x and so any solution of (8) satisfying the sign condition (SC) also satisfies the inhomogeneous equation

$$(14) \quad L_c \varepsilon(x) = -2f(x).$$

We note here that since f is piecewise constant and compactly supported it has a Fourier sine transform that can be calculated to be

$$(15) \quad \mathcal{F}_s[f](\kappa) = -\frac{1}{\sqrt{2\pi}} \frac{4 \sin^2\left(\frac{1}{2}\kappa\right)}{\kappa}.$$

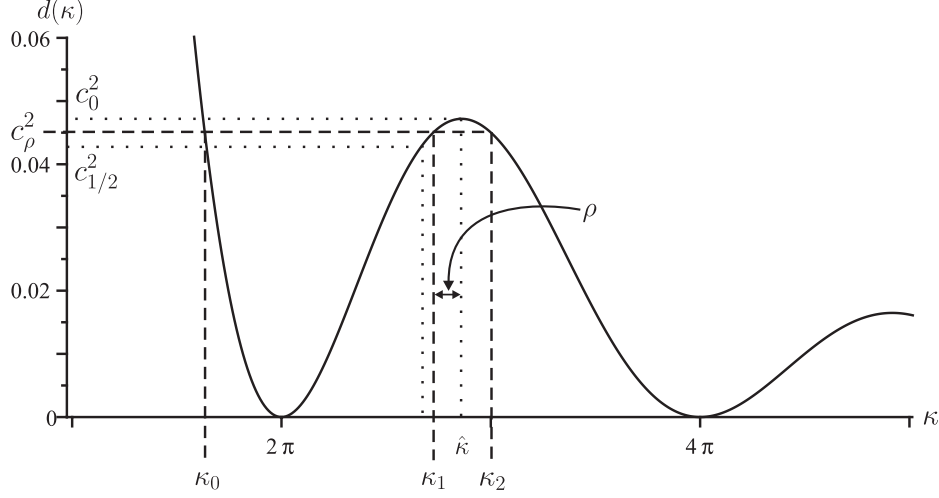


FIGURE 2. Key notation for this paper

The proof outline is as follows. Assume for contradiction that there exists a solution (1) that satisfies (SC) for the range of wave speeds considered here. The first step is to show that equation (14) has a solution. Secondly we then need to demonstrate that the solution we find violates (SC) and therefore cannot be a solution of the full equation. In a final step, since the solution we find in the first step is not unique, we demonstrate that any other distributional solution to (14) also fails (SC).

4. PROFILE-CORRECTOR METHOD

The profile-corrector method in [8] works as follows. Define an explicit *profile function*, called ε_{pr} , that is designed to remove the singularities in

$$(16) \quad \frac{\mathcal{F}[f](\kappa)}{D(\kappa)}.$$

Then show that ε_{pr} satisfies

$$(17) \quad L_c \varepsilon_{\text{pr}}(x) = -2f(x) + \Phi(x),$$

where $\Phi \in L^2(\mathbb{R})$. We then define the *corrector function*, denoted by ε_{cor} , as the solution to

$$(18) \quad L_c \varepsilon_{\text{cor}}(x) = \Phi(x).$$

Then $\varepsilon := \varepsilon_{\text{pr}} - \varepsilon_{\text{cor}}$ obviously solves (14). The advantage now being that Φ has much better properties than $-2f$, in particular, its Fourier transform has the same zeros as $D(\kappa)$ and hence no singularities. We may then demonstrate failure of the sign condition (SC) as follows. First we identify some points of the profile function where the sign condition is violated. Then we show that the $L^\infty(\mathbb{R})$ norm of ε_{cor} is sufficiently small as to not change the sign of ε in the neighbourhood of the points found in the first step.

The problem of integrating over singularities induced by zeros of the dispersion function is acknowledged in the physics literature. A *causality principle for steady-state* solution is introduced as a formal solution method [11]. In this approach one integrates along paths in the complex plane that avoid the singularities in solving (16), then considers the limit as the path approaches the real line. However, the representation of the solution as a formal sum makes verification of the sign condition difficult.

We define the profile function as follows. Suppose we have selected $\rho \in (\frac{1}{25}, \frac{1}{2})$ and obtained the wave speed c_ρ and the roots κ_i of $d(\kappa) = c_\rho^2$ for $i = 0, 1, 2$. Let α_i and $\beta_i > 0$ be real constants for $i = 0, 1, 2$ to be fixed later.

Adapting the approach of [8] we define a profile function as follows. First let us introduce an oscillating part as

$$(19) \quad \varepsilon_{\text{pr}}^{\text{osc}}(x) := \text{sign}(x) \left[\sum_{i=0}^2 \alpha_i \left(\frac{2 \sin^2(\frac{1}{2} \kappa_i x)}{\kappa_i^2} + \frac{1 - \exp(-\beta_i |x|)}{\beta_i^2} \right) \right].$$

The purpose of $\varepsilon_{\text{pr}}^{\text{osc}}$ is to capture the oscillating tails of the solution and join them smoothly at the origin. Note that $\varepsilon_{\text{pr}}^{\text{osc}} \in C^2(\mathbb{R})$ for all values of κ_i and β_i , $i = 0, 1, 2$. We then define a function with jumps in the second derivative at $x = -1, 0, 1$,

$$(20) \quad \varepsilon_{\text{pr}}^{\text{jump}}(x) := -\frac{1}{2c_\rho^2} \Delta_1 \left[\text{sign}(x) \frac{1}{4} |x|^2 \right].$$

The purpose of this function is that when added to the profile it compensates the jumps that occur in the right-hand side of (14). We are now in a position to define the profile function,

$$(21) \quad \varepsilon_{\text{pr}}(x) := \varepsilon_{\text{pr}}^{\text{osc}}(x) + \varepsilon_{\text{pr}}^{\text{jump}}(x).$$

Choosing the profile as an odd function in x allows us to use the Fourier sine transform throughout the remainder of the paper. The values for α_i and β_i are determined in Lemma 4.1, a plot of ε_{pr} for these values is included in Figure 3. In order to demonstrate that (SC) does not hold it is necessary to find a diverging sequence of points where the sign condition fails, since a solution of (18) allows for the solution ε to be modified in a neighbourhood of 0.

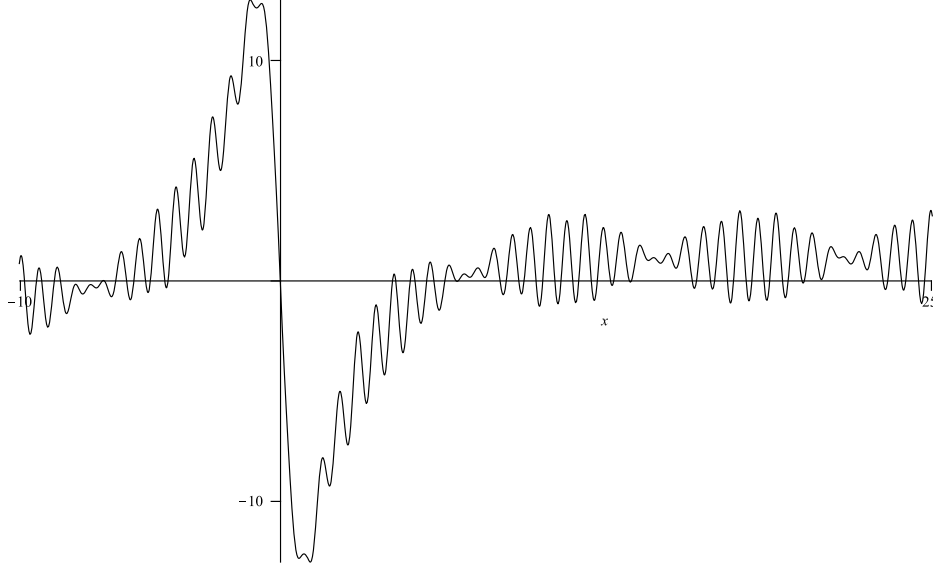


FIGURE 3. The function ε_{pr} for $-10 < x < 25$ with wave speed $c^2 = 0.045$, illustrating the failure of (SC)

As outlined in the introduction to this section, given the profile function defined above we need to show that there exists a function satisfying the corresponding corrector equation (18).

Lemma 4.1. *Let $\frac{1}{25} < \rho < \frac{1}{2}$. The profile function defined in (21) gives rise to a $\Phi \in L^2(\mathbb{R})$ as defined in (17). Furthermore, given Φ , (18) has a unique solution in $L^2(\mathbb{R})$.*

Proof. Fix $\frac{1}{25} < \rho < \frac{1}{2}$ and hence fix c_ρ^2 . The Fourier sine transform of $L_{c_\rho} \varepsilon_{\text{pr}}$ is

$$(22) \quad \mathcal{F}_s[L_{c_\rho} \varepsilon_{\text{pr}}](\kappa) = \sqrt{\frac{2}{\pi}} D(\kappa) \left(\sum_{i=0}^2 \frac{\alpha_i}{\kappa(\kappa_i^2 - \kappa^2)} \frac{\beta_i^2 + \kappa_i^2}{\beta_i^2 + \kappa^2} - \frac{4 \sin^2(\frac{1}{2}\kappa)}{\kappa} \frac{1}{c_\rho^2 \kappa^2} \right).$$

By (15), (17) and (22) it follows that

$$\begin{aligned}
 \mathcal{F}_s[\Phi](\kappa) &= \mathcal{F}_s[L_{c_\rho}\varepsilon_{\text{pr}}](\kappa) + 2\mathcal{F}_s[f](\kappa) \\
 (23) \quad &= \sqrt{\frac{2}{\pi}} \left\{ D(\kappa) \left(\sum_{i=0}^2 \frac{\alpha_i}{\kappa(\kappa_i^2 - \kappa^2)} \frac{\beta_i^2 + \kappa_i^2}{\beta_i^2 + \kappa^2} - \frac{4 \sin^2(\frac{1}{2}\kappa)}{c_\rho^2 \kappa^3} \right) - \frac{4 \sin^2(\frac{1}{2}\kappa)}{\kappa} \right\}.
 \end{aligned}$$

Obviously the only candidates for singularities in the Fourier sine transform of Φ are $\kappa \in \{0, \kappa_0, \kappa_1, \kappa_2\}$.

The singularities are all removable. From these observations we conclude that the Fourier sine transform of Φ is bounded as a function in κ . Since $\mathcal{F}_s[\Phi]$ is bounded and decays as a function in κ it follows that $\mathcal{F}_s[\Phi] \in L^2(\mathbb{R})$. Furthermore, since $\mathcal{F}[\Phi] = -i\mathcal{F}_s[\Phi] \in L^2(\mathbb{R})$ it follows from Parseval's identity that $\Phi \in L^2(\mathbb{R})$. It remains to show that, given Φ , (18) has a unique solution in $L^2(\mathbb{R})$. We make the following definitions

$$P(\kappa) := \prod_{j=0}^2 (\kappa_j^2 - \kappa^2) \quad \text{and} \quad p_i(\kappa) = \frac{P(\kappa)}{(\kappa_i^2 - \kappa^2)} \quad \text{for } i = 0, 1, 2.$$

We also define the rescaled variables $\ell_i := \kappa/\kappa_i$. Taking the Fourier sine transform of (18) and setting

$$\gamma_i^2 := \left(1 + \frac{\kappa_i^2}{\beta_i^2}\right)^{-1}$$

we find that

$$\begin{aligned}
 \mathcal{F}_s[\varepsilon_{\text{cor}}](\kappa) &= \frac{\mathcal{F}_s[\Phi](\kappa)}{D(\kappa)} \\
 &= \sqrt{\frac{2}{\pi}} \left\{ \left(\sum_{i=0}^2 \frac{\alpha_i}{\kappa(\kappa_i^2 - \kappa^2)} \frac{\beta_i^2 + \kappa_i^2}{\beta_i^2 + \kappa^2} - \frac{4 \sin^2(\frac{1}{2}\kappa)}{c_\rho^2 \kappa^3} \right) - \frac{4 \sin^2(\frac{1}{2}\kappa)}{\kappa D(\kappa)} \right\} \\
 &= \sqrt{\frac{2}{\pi}} \left\{ \frac{1}{\kappa P(\kappa)} \left(\sum_{i=0}^2 \alpha_i p_i(\kappa) \frac{\beta_i^2 + \kappa_i^2}{\beta_i^2 + \kappa^2} - \frac{(4 \sin^2(\frac{1}{2}\kappa))^2 \kappa^2 P(\kappa)}{c_\rho^2 \kappa^4 D(\kappa)} \right) \right\} \\
 (24) \quad &= \sqrt{\frac{2}{\pi}} \frac{1}{\kappa P(\kappa)} \left(\sum_{i=0}^2 \frac{\alpha_i p_i(\kappa)}{\ell_i^2 + \gamma_i^2 (1 - \ell_i^2)} - \frac{1}{c_\rho^2} \left(\frac{2 \sin(\frac{1}{2}\kappa)}{\kappa} \right)^4 \frac{\kappa^2 P(\kappa)}{D(\kappa)} \right).
 \end{aligned}$$

As before with the Fourier sine transform of Φ we see that the only candidates for singularities in (24) are $\kappa \in \{0, \kappa_0, \kappa_1, \kappa_2\}$. Taking the limit $\kappa \rightarrow \kappa_i$ for any $i = 0, 1, 2$ and applying L'Hôpital's rule, noting that the range of ρ ensures D has roots of single multiplicity, we find that

$$(25) \quad \lim_{\kappa \rightarrow \kappa_i} \left(\sum_{i=0}^2 \frac{\alpha_i p_i(\kappa)}{\ell_i^2 + \gamma_i^2 (1 - \ell_i^2)} - \frac{1}{c_\rho^2} \left(\frac{2 \sin(\frac{1}{2}\kappa)}{\kappa} \right)^4 \frac{\kappa^2 P(\kappa)}{D(\kappa)} \right) = p_i(\kappa_i) \left(\alpha_i - \frac{c_\rho^2 \kappa_i^3}{c_\rho^2 \kappa_i - \sin(\kappa_i)} \right),$$

which vanishes if we set

$$(26) \quad \alpha_i := \frac{c_\rho^2 \kappa_i^3}{c_\rho^2 \kappa_i - \sin(\kappa_i)}.$$

The function in (25) therefore has a continuous extension at κ_i and in particular the continuous extension has a root at κ_i . Hence $\mathcal{F}_s[\varepsilon_{\text{cor}}]$ is bounded for $\kappa \in \{\kappa_0, \kappa_1, \kappa_2\}$. To show that $\mathcal{F}_s[\varepsilon_{\text{cor}}]$ is bounded as $\kappa \rightarrow 0$ we need to apply L'Hôpital's rule twice to find that (24) becomes

$$\sum_{i=0}^2 \frac{\alpha_i}{\kappa_i^2 \gamma_i^2} - \frac{1}{c_\rho^2(1 - c_\rho^2)} = \sum_{i=0}^2 \frac{\text{sign}(\alpha_i)}{c_\rho^2(1 - c_\rho^2)} - \frac{1}{c_\rho^2(1 - c_\rho^2)} = 0,$$

if we take $\beta_i > 0$ to satisfy

$$(27) \quad \left(1 + \frac{\kappa_i^2}{\beta_i^2}\right)^{-1} := |\alpha_i| \frac{c_\rho^2(1 - c_\rho^2)}{\kappa_i^2}.$$

and the fact that $\alpha_0, \alpha_2 > 0$ and $\alpha_1 < 0$. To show that $\alpha_0, \alpha_2 > 0$ and $\alpha_1 < 0$ we define a function α as

$$(28) \quad \alpha(\kappa) := \frac{d^2(\kappa)\kappa^3}{d^2(\kappa)\kappa - \sin(\kappa)},$$

which has the property that $\alpha(\kappa_i) = \alpha_i$ for a fixed ρ as $c_\rho^2 = d^2(\kappa_i)$. Recall from equation (12) that for our range of c_ρ^2 it follows that $\kappa_i \in W_i$, $i = 0, 1, 2$. Then examining α on these intervals, we observe that $\alpha_0, \alpha_2 > 0$ and $\alpha_1 < 0$, see Figure 4. Since α is a bounded regular function on W_i , $i = 0, 1, 2$, it is also straightforward to prove the sign distribution rigourously [13].

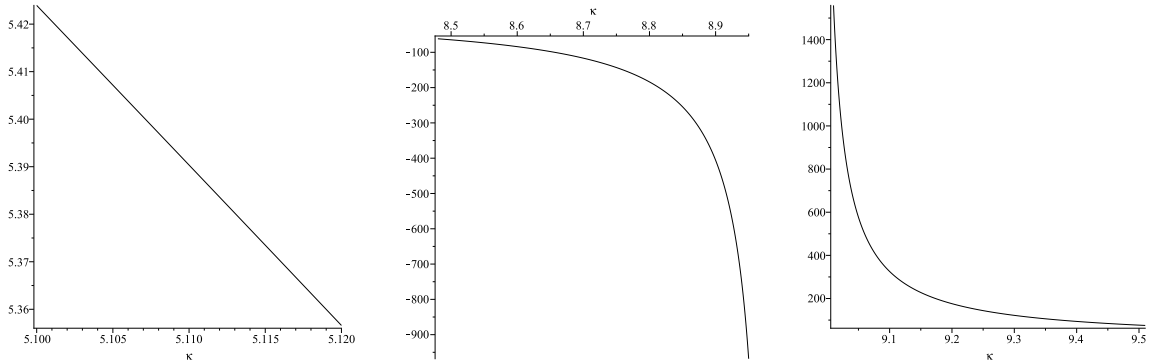


FIGURE 4. The function α which generates the constants α_i on the intervals W_0 (left), W_1 (centre) and W_2 (right)

It is important to also ensure that the β_i are well defined. We will show now that (27) and our plot of α that $|\alpha(\kappa)| \rightarrow \infty$ as $\kappa \rightarrow \hat{\kappa}$ implies that the β_i become complex, for sufficiently small ρ . As with α_i it is possible to define a function β that satisfies

$$(29) \quad \left(1 + \frac{\kappa^2}{\beta(\kappa)^2}\right)^{-1} := |\alpha(\kappa)| \frac{d^2(\kappa)(1 - d^2(\kappa))}{\kappa^2}.$$

The function β is only real valued when the right hand side of (30) is less than 1, or equivalently

$$(30) \quad \frac{\kappa^2}{\beta(\kappa)^2} := \frac{\kappa^2}{d^2(\kappa)(1 - d^2(\kappa)) |\alpha(\kappa)|} - 1 > 0.$$

We plot the right hand side of (30), see Figure 5, which is bounded and regular on the intervals W_i , $i = 0, 1, 2$ to verify positivity. Again, the positivity can be proved rigourously, see [13].

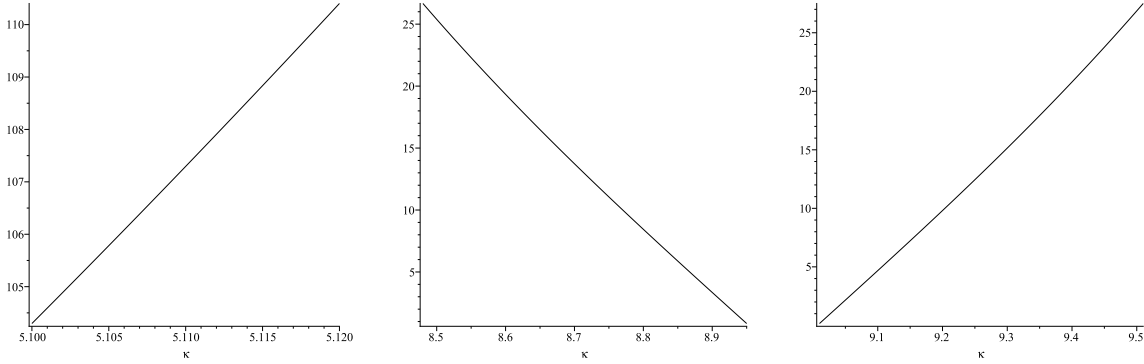


FIGURE 5. The function β which generates the constants β_i on the intervals W_0 (left), W_1 (centre) and W_2 (right)

We have shown that $\mathcal{F}_s[\varepsilon_{\text{cor}}]$ is bounded at all of the potential singularities and therefore bounded on \mathbb{R} as a function in κ . Since $\mathcal{F}_s[\varepsilon_{\text{cor}}]$ is bounded and decays as a function in κ it follows that $\mathcal{F}_s[\varepsilon_{\text{cor}}] \in L^2(\mathbb{R})$. Furthermore, since $\mathcal{F}[\varepsilon_{\text{cor}}] = -i\mathcal{F}_s[\varepsilon_{\text{cor}}] \in L^2(\mathbb{R})$ it follows from Parseval's identity that $\Phi \in L^2(\mathbb{R})$ and uniquely satisfies (18). \square

Note that in the above proof the following fact was demonstrated.

Corollary 1. *For every $\frac{1}{25} < \rho < \frac{1}{2}$ it follows that $\alpha_0, \alpha_2 > 0$ and $\alpha_1 < 0$.*

The following lemma shows that the tails of the corrector decay as $x \rightarrow \pm\infty$.

Lemma 4.2. *Let $\frac{1}{25} < \rho < \frac{1}{2}$. For all $\delta > 0$ the set $\{x : |\varepsilon_{\text{cor}}(x)| \geq \delta\}$ is compact.*

Proof. We have that $\mathcal{F}[\varepsilon'_{\text{cor}}](\kappa) = i\kappa\mathcal{F}[\varepsilon_{\text{cor}}](\kappa) = \kappa\mathcal{F}_s[\varepsilon_{\text{cor}}](\kappa)$ and therefore

$$\mathcal{F}[\varepsilon'_{\text{cor}}](\kappa) = \sqrt{\frac{2}{\pi}} \left\{ \frac{1}{P(\kappa)} \left(\sum_{i=0}^2 \frac{\alpha_i p_i(\kappa)}{\ell_i^2 + \gamma_i^2(1 - \ell_i^2)} - \frac{1}{c_\rho^2} \left(\frac{2 \sin(\frac{1}{2}\kappa)}{\kappa} \right)^4 \frac{\kappa^2 P(\kappa)}{D(\kappa)} \right) \right\}.$$

We can see that the pole at $\kappa = 0$ is removeable and the remaining potential poles are handled by the choice of α_i $i = 0, 1, 2$, as before. Then $\mathcal{F}[\varepsilon'_{\text{cor}}]$ is bounded and decays as a function in κ , hence $\mathcal{F}[\varepsilon'_{\text{cor}}] \in L^2(\mathbb{R})$, and therefore by the Plancherel theorem we have that $\varepsilon'_{\text{cor}} \in L^2(\mathbb{R})$. Therefore $\varepsilon_{\text{cor}} \in H^1(\mathbb{R})$ and by the Sobolev embedding theorem [5, Theorem 8.54] $\varepsilon_{\text{cor}}(x) \rightarrow 0$ as $x \rightarrow \pm\infty$. \square

The next result determines explicitly all bounded solutions to the homogeneous version of (14).

Lemma 4.3. *Let $\frac{1}{25} < \rho < \frac{1}{2}$ and $\varepsilon \in L^\infty(\mathbb{R})$. Then $L_{c_\rho}\varepsilon = 0$ if and only if*

$$\varepsilon \in K := \text{span} \left(\{1\} \cup \{\cos(\kappa_i x)\}_{i=0}^2 \cup \{\sin(\kappa_i x)\}_{i=0}^2 \right).$$

Proof. This follows by taking the Fourier transform in the sense of tempered distributions. Since the roots of the dispersion function are isolated, it immediately follows $\mathcal{F}[\varepsilon]$ is the sum of Dirac delta. The result follows. \square

Since (14) is an inhomogeneous linear equation, the solution to (14) is only unique modulo K . From this observation it is clear that even if one shows that ε fails the sign condition (SC) then it may still satisfy it if we add a suitable combination of functions from K . Schwetlick and Zimmer show [9] that in addition to the point symmetric wave found in [8], there also exists a family of asymmetric heteroclinic travelling waves for the same range of wave speeds. This is achieved by adding suitable combinations of functions from K and showing that the sign condition (SC) is still satisfied.

The solution ε can be expressed in the form

$$\varepsilon(x) = \text{sign}(x)\varepsilon_{\text{tail}}(x) + \varepsilon_{\text{decay}}(x),$$

where $\varepsilon_{\text{decay}}(x) \rightarrow 0$ as $x \rightarrow \pm\infty$ and

$$\varepsilon_{\text{tail}}(x) := \sum_{i=0}^2 \alpha_i \left(\frac{1}{\kappa_i^2} + \frac{1}{\beta_i^2} \right) - \sum_{i=0}^2 \frac{\alpha_i}{\kappa_i^2} \cos(\kappa_i x) - \frac{1}{c_\rho^2}.$$

The next lemma demonstrates that every solution of (14) fails to satisfy the sign condition (SC).

Lemma 4.4. *Let $\frac{1}{25} < \rho < \frac{1}{2}$ and suppose that there exists a point $x \in \mathbb{R}$ where $\varepsilon_{\text{tail}}(x) < -\frac{1}{10}$. Then for any $\eta \in K$ (defined in Lemma 4.3) one of the following holds:*

(a) *there exists a sequence $\{z_n\}_{n=1}^\infty \subset \mathbb{R}$ with $z_n \rightarrow \infty$ such that $\varepsilon_{\text{tail}}(z_n) + \eta(z_n) < -\frac{1}{20}$, or,*

(b) *there exists a sequence $\{z_n\}_{n=1}^\infty \subset \mathbb{R}$ with $z_n \rightarrow -\infty$ such that $-\varepsilon_{\text{tail}}(z_n) + \eta(z_n) > \frac{1}{20}$.*

Proof. Suppose for contradiction that both (a) and (b) are not satisfied. Then there exists x, y such that $-\infty < y < 0 < x < \infty$, $\varepsilon_{\text{tail}}(z) + \eta(z) \geq -\frac{1}{20}$ for every $z > x$ and $-\varepsilon_{\text{tail}}(z) + \eta(z) \leq \frac{1}{20}$ for every $z < y$. Since $\pm\varepsilon_{\text{tail}} + \eta$ is quasi-periodic, it follows that $\varepsilon_{\text{tail}}(z) + \eta(z) \geq -\frac{1}{20}$ and $-\varepsilon_{\text{tail}}(z) + \eta(z) \leq \frac{1}{20}$ for all $z \in \mathbb{R}$. Consequently $\varepsilon_{\text{tail}} \geq -\frac{1}{20}$ for all $z \in \mathbb{R}$, a contradiction to the hypotheses of the lemma. \square

The proof that $\varepsilon_{\text{tail}}$ attains a negative value is contained in Section 5 to maintain the flow of this argument.

We are now in a position to prove the main theorem.

Proof of Theorem 3.1. Fix $\frac{1}{25} < \rho < \frac{1}{2}$ and suppose the solution ε to (8) satisfies the sign condition (SC). Then, decomposing $\varepsilon = \varepsilon_{\text{pr}} - \varepsilon_{\text{cor}}$ with ε_{pr} as in (21) gives rise to a corrector function ε_{cor} by Lemma 4.1. It follows that this is only unique modulo K and find that the general solution to (14) is $\varepsilon + \eta$, $\eta \in K$.

By Lemma 4.2 we have that $|\varepsilon_{\text{cor}}(x)| \rightarrow 0$ as $|x| \rightarrow \infty$ so there is a $M \in \mathbb{R}$ such that if $|x| > M$ then $|\varepsilon_{\text{cor}}(x)| < \frac{1}{30}$. By Lemma 4.4 there exists a sequence $\{z_n\}_{n=1}^\infty \subset \mathbb{R}$ with $|z_n| \rightarrow \infty$ as $n \rightarrow \infty$ such that either $\varepsilon_{\text{pr}}(z_n) + \eta(z_n) < -\frac{1}{20}$ or $\varepsilon_{\text{pr}}(z_n) + \eta(z_n) > \frac{1}{20}$ for each $n \in \mathbb{N}$. Choose N sufficiently large so that $|z_N| > M$. Then either

$$\varepsilon(z_N) < |\varepsilon_{\text{cor}}(z_N)| - \frac{1}{20} < -\frac{1}{60} \quad \text{if } z_N > 0$$

or

$$\varepsilon(z_N) > -|\varepsilon_{\text{cor}}(z_N)| + \frac{1}{20} > \frac{1}{60} \quad \text{if } z_N < 0.$$

Therefore for each solution of (14) we can find a point where the sign condition (SC) is not satisfied. This contradicts the assumption that the sign condition holds. \square

5. SIGN FAILURE OF THE PROFILE

The purpose of this section is to show that $\varepsilon_{\text{tail}}$ attains a negative value. Let $\frac{1}{25} < \rho < \frac{1}{2}$ and define

$$(31) \quad \kappa_{\sigma} := \frac{\kappa_2 + \kappa_1}{2}, \quad \kappa_{\delta} := \frac{\kappa_2 - \kappa_1}{2}.$$

The next proposition characterises the tail part for large values of $|x|$.

Proposition 1. *For $\frac{1}{25} < \rho < \frac{1}{2}$ there exists a point $X \in \mathbb{R}$ such that $\varepsilon_{\text{tail}}(X) < -\frac{1}{10}$.*

Proof. By simple manipulation,

$$(32) \quad \begin{aligned} \varepsilon_{\text{tail}}(x) &= \sum_{i=0}^2 \alpha_i \left(\frac{1}{\kappa_i^2} + \frac{1}{\beta_i^2} \right) - \sum_{i=0}^2 \frac{\alpha_i}{\kappa_i^2} \cos(\kappa_i x) - \frac{1}{c_{\rho}^2} \\ &= \sum_{i=0}^2 \alpha_i \left(\frac{1}{\kappa_i^2} + \frac{1}{\beta_i^2} \right) + \sum_{i=0}^2 \left| \frac{\alpha_i}{\kappa_i^2} \right| \cos(\kappa_i x + \theta_i) - \frac{1}{c_{\rho}^2} \end{aligned}$$

where $\theta_0, \theta_2 = -\pi$ and $\theta_1 = 0$, taking into account Corollary 1. Substituting (27) into (32), it follows that

$$\varepsilon_{\text{pr}}(x) = \sum_{i=0}^2 \left(\frac{\alpha_i}{|\alpha_i| c_{\rho}^2 (1 - c_{\rho}^2)} \right) + \sum_{i=0}^2 \left| \frac{\alpha_i}{\kappa_i^2} \right| \cos(\kappa_i x + \theta_i) - \frac{1}{c_{\rho}^2}$$

and again by Corollary 1

$$(33) \quad \varepsilon_{\text{pr}}(x) = \frac{1}{1 - c_{\rho}^2} + \sum_{i=0}^2 \left| \frac{\alpha_i}{\kappa_i^2} \right| \cos(\kappa_i x + \theta_i).$$

After further trigonometric manipulation and using the definitions in (31), (33) becomes

$$(34) \quad \begin{aligned} \varepsilon_{\text{pr}}(x) &= \frac{1}{1 - c_{\rho}^2} + \left| \frac{\alpha_0}{\kappa_0^2} \right| \cos(\kappa_0 x - \pi) \\ &\quad + \left(\left| \frac{\alpha_1}{\kappa_1^2} \right| + \left| \frac{\alpha_2}{\kappa_2^2} \right| \right) \cos(\kappa_{\sigma} x - \frac{\pi}{2}) \cos(\kappa_{\delta} x - \frac{\pi}{2}) \\ &\quad + \left(\left| \frac{\alpha_1}{\kappa_1^2} \right| - \left| \frac{\alpha_2}{\kappa_2^2} \right| \right) \sin(\kappa_{\sigma} x - \frac{\pi}{2}) \sin(\kappa_{\delta} x - \frac{\pi}{2}). \end{aligned}$$

Suppose for now that there exists a point X such that: $|\alpha_0/\kappa_0^2| \cos(\kappa_0 X - \pi) \leq 0$, $\cos(\kappa_\sigma X - \frac{\pi}{2}) = 1$, and the point X is within a distance of $4\pi/\kappa_\sigma$ of a minimum point of $\cos(\kappa_\delta x - \frac{\pi}{2})$. Evaluating (34) at X we find that

$$(35) \quad \varepsilon_{\text{pr}}(X) = \frac{1}{1 - c_\rho^2} + \left(\left| \frac{\alpha_1}{\kappa_1^2} \right| + \left| \frac{\alpha_2}{\kappa_2^2} \right| \right) \cos(\kappa_\delta X - \frac{\pi}{2}),$$

where the product of sines vanishes due to the choice of X . Using a second order Taylor expansion of $\cos(\kappa_\delta x - \frac{\pi}{2})$ around the minimum point y and the fact that $|y - X| \leq 4\pi/\kappa_\sigma$, it follows that

$$(36) \quad \begin{aligned} \varepsilon_{\text{pr}}(z) &= \frac{1}{1 - c_\rho^2} - \left(\left| \frac{\alpha_1}{\kappa_1^2} \right| + \left| \frac{\alpha_2}{\kappa_2^2} \right| \right) (1 - \frac{1}{2}(y - X)^2) \\ &\leq \frac{1}{1 - c_\rho^2} - \left(\left| \frac{\alpha_1}{\kappa_1^2} \right| + \left| \frac{\alpha_2}{\kappa_2^2} \right| \right) \left(1 - 8\pi^2 \frac{\kappa_\delta^2}{\kappa_\sigma^2} \right). \end{aligned}$$

Hence the result follows if

$$\frac{1}{1 - c_\rho^2} - \left(\left| \frac{\alpha_1}{\kappa_1^2} \right| + \left| \frac{\alpha_2}{\kappa_2^2} \right| \right) \left(1 - 8\pi^2 \frac{\kappa_\delta^2}{\kappa_\sigma^2} \right) \leq -\frac{1}{10},$$

or equivalently,

$$(37) \quad \left(1 - 8\pi^2 \frac{\kappa_\delta^2}{\kappa_\sigma^2} \right)^{-1} \left(\frac{1}{1 - c_\rho^2} + \frac{1}{10} \right) \leq \left| \frac{\alpha_1}{\kappa_1^2} \right| + \left| \frac{\alpha_2}{\kappa_2^2} \right|,$$

(note that $8\pi^2(\kappa_\delta^2/\kappa_\sigma^2) \ll 1$ by the bounds on κ_i). A calculation shows that

$$(38) \quad \left(1 - 8\pi^2 \frac{\kappa_\delta^2}{\kappa_\sigma^2} \right)^{-1} \left(\frac{1}{1 - c_\rho^2} + \frac{1}{10} \right) < 1.57.$$

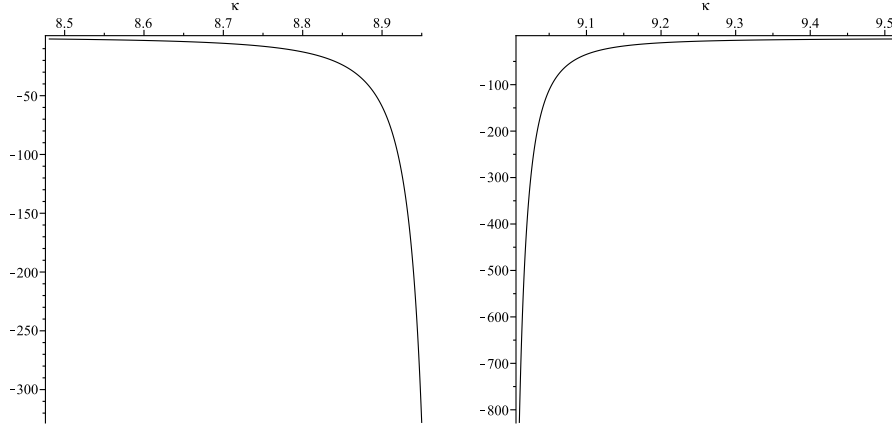
The upper bound (38) follows by using the numerical bounds on the roots of the dispersion function. Recall from (28) that $\alpha_i = \alpha(\kappa_i)$. The function $\alpha(\kappa)/\kappa^2$ is bounded, regular and monotone on W_1 and W_2 , which can be either verified analytically [13] or seen from Figure 6, and hence by the same numerical bounds on the possible values for κ_1 and κ_2 it follows that

$$\left| \frac{\alpha_1}{\kappa_1^2} \right| + \left| \frac{\alpha_2}{\kappa_2^2} \right| \geq \min_{W_1} \left| \frac{\alpha(\kappa)}{\kappa^2} \right| + \min_{W_2} \left| \frac{\alpha(\kappa)}{\kappa^2} \right| > 1.60.$$

Hence (37) holds.

It remains to show that the point X exists. Let

$$x := \frac{\pi}{2\kappa_\delta} \text{ and } z_n := \frac{2\pi}{\kappa_\sigma} n + \frac{\pi}{2\kappa_\sigma}, \text{ for } n \in \mathbb{N}.$$

FIGURE 6. Plots of $(\alpha(\kappa)/\kappa^2)'$ over W_1 (left) and W_2 (right)

It is clear that $\cos(\kappa_\delta x - \frac{\pi}{2}) = -1$ and $\cos(\kappa_\sigma z_n - \frac{\pi}{2}) = 1$ for every n . Since $\cos(\kappa_\sigma x - \frac{\pi}{2})$ is $2\pi/\kappa_\sigma$ -periodic that there exists $m \in \mathbb{N}$ such that $0 \leq x - z_m < 2\pi/\kappa_\sigma$. See Figure 7 for a diagrammatic explanation of the notation; the solid and dashed intervals at the bottom indicates the intervals where $|\alpha_0/\kappa_0^2| \cos(\kappa_0 x - \pi)$ has a fixed sign and the dashed curve is $(|\alpha_1/\kappa_1^2| + |\alpha_2/\kappa_2^2|) \cos(\kappa_\delta x - \frac{\pi}{2})$. Furthermore, it is obvious that $0 \leq z_{m+1} - x < 2\pi/\kappa_\sigma$ and $2\pi/\kappa_\sigma \leq z_{m+2} - x < 4\pi/\kappa_\sigma$. It remains to show that there exists an $X \in \{z_m, z_{m+1}, z_{m+2}\}$ such that $|\alpha_0/\kappa_0^2| \cos(\kappa_0 X - \pi) \leq 0$.

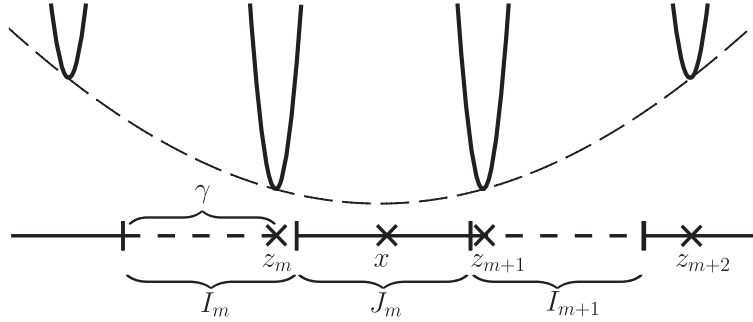


FIGURE 7. The notation used in the proof of Proposition 1

If $|\alpha_0/\kappa_0^2| \cos(\kappa_0 z_m - \pi) \leq 0$ then no further work is required. Otherwise one concludes that there exists $p \in \mathbb{N}$ such that

$$z_m = \frac{1}{\kappa_0} \left(\frac{\pi}{2} + \pi \right) + \frac{\pi(2p+1)}{\kappa_0} + \gamma,$$

for $\gamma \in (0, \pi/\kappa_0)$. This holds since we can write $(0, \infty) = (\cup_{q \in \mathbb{N}_0} I_q) \cup (\cup_{q \in \mathbb{N}_0} J_q) \cup I$, where

$$I := \left(0, \frac{3\pi}{2\kappa_0}\right), \quad I_q := \frac{\pi(2q+1)}{\kappa_0} + \frac{3\pi}{2\kappa_0} + \left(0, \frac{\pi}{\kappa_0}\right)$$

and

$$J_q := \frac{2\pi q}{\kappa_0} + \frac{3\pi}{2\kappa_0} + \left[0, \frac{\pi}{\kappa_0}\right].$$

A simple calculation demonstrates that $\cos(x) > 0$ on I_q and $\cos(x) \leq 0$ on J_q . Since, by definition,

$$\begin{aligned} z_{m+1} &= z_m + \frac{2\pi}{\kappa_\sigma} \\ &= \frac{3\pi}{2\kappa_0} + \frac{2\pi(p+1)}{\kappa_0} + \gamma + \frac{2\pi}{\kappa_\sigma} - \frac{\pi}{\kappa_0}, \end{aligned}$$

it follows that $|\alpha_0/\kappa_0^2| \cos(\kappa_0 z_{m+1} - \pi) \leq 0$, or equivalently $z_{m+1} \in J_{p+1}$, if

$$(39) \quad 0 \leq \gamma + \frac{2\pi}{\kappa_\sigma} - \frac{\pi}{\kappa_0} \leq \frac{\pi}{\kappa_0}.$$

Since we have explicit bounds for γ , κ_0 and κ_σ from the considerations in Lemma 4.1 a calculation shows that the lower bound in (39) holds uniformly in ρ . The upper bound is not necessarily satisfied and therefore we can only be sure that $|\alpha_0/\kappa_0^2| \cos(\kappa_0 z_{m+1} - \pi) \leq 0$ if $\gamma \leq 2\pi/\kappa_0 - 2\pi/\kappa_\sigma$. If we know $\gamma \leq 2\pi/\kappa_0 - 2\pi/\kappa_\sigma$ then we have found the required point, otherwise $2\pi/\kappa_0 - 2\pi/\kappa_\sigma < \gamma < \pi/\kappa_0$, the upper bound arising from the definition of γ . By definition,

$$\begin{aligned} z_{m+2} &= z_m + \frac{4\pi}{\kappa_\sigma} \\ &= \frac{2\pi(p+2)}{\kappa_0} + \gamma + \frac{4\pi}{\kappa_\sigma} - \frac{3\pi}{2\kappa_0}. \end{aligned}$$

Proceeding as before, we have that it follows that $|\alpha_0/\kappa_0^2| \cos(\kappa_0 z_{m+2} - \pi) \leq 0$, equivalently $z_{m+2} \in J_{p+2}$, if

$$(40) \quad 0 \leq \gamma + \frac{4\pi}{\kappa_\sigma} - \frac{3\pi}{\kappa_0} \leq \frac{\pi}{\kappa_0}.$$

which is equivalent to

$$(41) \quad \frac{3\pi}{\kappa_0} - \frac{4\pi}{\kappa_\sigma} < \gamma < \frac{4\pi}{\kappa_0} - \frac{4\pi}{\kappa_\sigma}.$$

Using the numerical bounds on the roots of the dispersion function from Lemma 4.1 and the assumption that $2\pi/\kappa_0 - 2\pi/\kappa_\sigma < \gamma < \pi/\kappa_0$ one can show that (41) holds. What we have demonstrated is that there is at least one point in $\{z_m, z_{m+1}, z_{m+2}\}$ such that $|\alpha_0/\kappa_0^2| \cos(\kappa_0 z_{m+i} - \pi) \leq 0$. Denote this point as X . \square

6. DISCUSSION

Here we have demonstrated that at wave speeds much less than the speed of sound, there are no travelling wave solutions that have bounded strain making a single transition between harmonic potential wells. In particular, we have shown that the solutions obtained in [8, 9] do not exist for the chosen significantly lower wave speeds. This confirms that for this model, the conjecture by Peyrard and Kruskal in [7] holds true and falls in line with the experimental observations of Förster and Scheil [4].

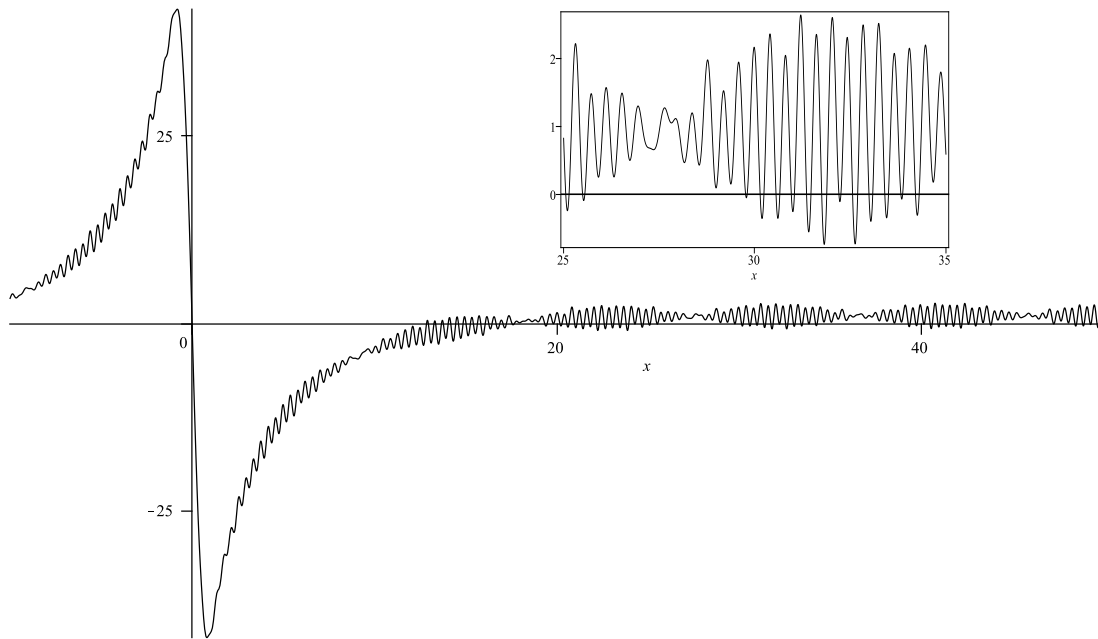


FIGURE 8. The function ε_{pr} for $-10 < x < 50$ with wave speed $c^2 = 0.016$. (Inset) A zoom view for $25 < x < 35$ illustrating the failure of (SC)

The main feature of the proof is that when the wave speed is low enough one can have two roots that become arbitrarily close together; then the contributions from the kernel function resonate, causing the failure of the sign condition. One can show that Lemmata 4.1, 4.2 and 4.3 hold when $D(\kappa)$ has an arbitrary number of roots, with obvious modifications. The key difficulty to determining a rigorous proof for lower wave speeds is showing the equivalent of Lemma 4.4, due to the lack of information regarding the commensurability of

the roots of the dispersion function. Specifically, should one be able to prove that the set of positive roots to the dispersion function is linearly independent over the integers then one can prove an analogue of 4.4 using Kronecker's Theorem for simultaneous Diophantine approximation [1, Sections 7.4 and 7.5]. By studying the profile function numerically for wave speeds corresponding to more than three roots we observe that the nonexistence of heteroclinic travelling waves persists. For instance, Figure 8 contains a plot of the case when $c^2 = 0.016$, a wave speed that corresponds to 5 distinct roots. The plot suggests that the sign condition fails in this case.

It may be possible that a certain combination of kernel functions, once added to a generalised version of the corresponding profile function, cancel the resonances generated and enable the existence of a single interface travelling wave solution. We expect, however, for wave speeds close to those corresponding to a double zero of the dispersion function that this is not the case, as we have seen here. Should one be able to prove this then one would find that there exists a sequence of intervals converging to 0 such that the same type of nonexistence result we obtain holds.

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